Estimating the Unknown Time Delay in Chemical Processes

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Abstract

Although time delay is an important element in both system identification and control performance assessment, its computation remains elusive. This paper proposes the application of a least squares support vector machines driven approach to the problem of determining constant time delay for a chemical process. The approach consists of two steps, where in the first step the state of the system and its derivative are approximated based on the LS-SVM model. The second stage consists of modeling the delay term and estimating the unknown model parameters as well as the time delay of the system. Therefore the proposed approach avoids integrating the given differential equation that can be computationally expensive. This time delay estimation method is applied to both simulation and experimental data obtained from a continuous, stirred, heated tank. The results show that the proposed method can provide accurate estimates even if significant noise or unmeasured additive disturbances are present.

Key words: Input-delay system, least squares support vector machines, continuous stirred tank, open and closed-loop identification

1. Introduction

The rapid growth and development of new chemical processes involves a need for effective, safe, and efficient methods for understanding and assessing their performance. The general framework for understanding the process, often called system identification, is a well-developed field [9, 21]. Similarly, performance assessment of the process has been well developed [19, 8, 10]. However, one area within these two frameworks that still requires further research is that of effective time delay determination. In system identification, a time delay is often assumed to be known *a priori* or determined using auxiliary methods, such as a step test or the cross-correlation method [17]. Similarly, many performance assessment methods, such as the Harris index, require the time delay to be known beforehand in order to effectively implement the assessment. This need for the time delay means that such a method can only rarely be implemented in industry due to the inability to obtain the relevant information [19]. This problem is especially acute in closed-loop process operation, that is, when a chemical process is being actively controlled by a controller. In such cases, many of the previously developed methods do not apply due to the correlation between the input and outputs signals, introduced by the controller.

Time delay estimation can be divided into four broad categories [4]: time-delay approximation methods, explicit time-delay parameter methods, area and moment methods, and finally, higher-order statistics methods. Time-delay approximation methods convert or project the given input and output signals into another basis from which a process model can be estimated. Using the estimated process model, the time delay can be back calculated. Of the available methods, the most common methods are the various Laguerre-domain based approximation methods. The explicit time-delay parameter methods seek to estimate the time delay directly with all the other parameters in the model. The most common approach is to assume a high-order autoregressive model with exogenous input (ARMAX) with varying time delays and select the time delay that provides the best overall fit as the time delay for the model. This approach

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is implemented in MATLAB's DELAYEST function and hence is often used in practical cases. However, although it can provide decent results for both open- and closed-loop cases, it does require the user to know at least approximately the range over which the time delays could vary. Furthermore, selecting an appropriate higher order model can be an issue as it can slow down the brute force search tremendously. The area and moment methods seek to determine the delay by examining either step or impulse response characteristics of the observed input and output signals and fitting an appropriate signal. It can be noted that in this approach there are two main steps: first, the desired response coefficients must be estimated and then the time delay extracted. Often the extraction of the time delay is performed visually since only a small data set is being used. The most common such methods are the various methods which seek to determine the cross-correlation or impulse coefficients between the input and output signals to determine the estimated time delay [17, 4]. The time delay is inferred by determining which of the computed cross-correlation lags is nonzero. Although this approach can provide very accurate results, it does require that the error be uncorrelated with the inputs and outputs and that the input be a white noise signal. In practice, this implies that this method only applies for open-loop processes driven by white noise or pseudorandom binary signals, which have properties similar to white noise [7]. Time delay methods based on higher order statistics are rarely used for industrial data since it can be complicated to compute the required values.

An active area of research is the development of methods to extend the explicit time delay estimation methods to handle more complex situation that involve solving the exact differential equations given all the available information and, thus, relatively easily obtain the optimal time delay. However, at each iteration, it is necessary to integrate the differential equation, which can be a computationally intensive task. Recently, with the expansion and development of new methods for rapid computation and implementation of the various time-delay optimization methods, a potentially new approach to time delay estimation has been proposed. Mehrkanoon *et al.* [14] proposed an approach based on least squares support vector machines (LS-SVM) for estimating the time delay given the observational data. Support Vector Machines (SVMs) are a powerful methodology for solving pattern recognition and function estimation problems [23], which solves the dual quadratic programming problem. LS-SVMs have been applied to function estimation, classification, problems in unsupervised learning and others [22]. The LS-SVM problem formulation involves equality, instead of inequality constraints and employs a quadratic loss function. Training of the model in the dual is then done by solving a set of linear equations. The method converts the parameter estimation problem into an algebraic optimization problem and, thus, does not require repeated numerical integration of the system. The ability of LS-SVM to produce a continuous output is used to estimate the state and its derivative. This information is then cast into an optimization problem that seeks to determine the time delay.

Therefore, given the potential suitability of this approach to chemical engineering application, the objectives of this paper are: to develop and understand the least squares support vector machine approach for time delay estimation in the context of chemical engineering examples; to investigate the behaviour and properties of this method using simulations of a heated tank; and to apply the method to experimental data obtained from running a pilot scale heated tank. In both cases, open- and closed-loop cases will be considered and the results compared. For the closed-loop case, two further subcases will be considered depending on whether or not the reference signal changes its value during the course of operation.

2. Overview of LS-SVM regression

Consider a given training set $\{t_i, y_i\}_{i=1}^N$ with input data $t_i \in \mathbb{R}^d$ and output data $y_i \in \mathbb{R}$. In the LS-SVM framework, one assumes that the underlying function describing the relation between input and output of the system has the following form:

$$y(t) = w^T \varphi(t) + b. \tag{1}$$

where $\varphi(\cdot) : \mathbb{R}^d \to \mathbb{R}^h$ is the feature map and h is the dimension of the feature space. Thanks to the nonlinear feature map, the data are embedded into a feature space and the optimal solution is sought in that space by minimizing the residual between the model outputs and the measurements. To this end, one formulates the following optimization problem known as primal LS-SVM formulation [22]:

$$
\begin{aligned}
\underset{w,b,e}{\text{minimize}} \quad & \frac{1}{2}w^T w + \frac{\gamma}{2}e^T e \\
\text{subject to} \quad & y_i = w^T \varphi(t_i) + b + e_i, \quad i = 1, ..., N,
\end{aligned} \tag{2}
$$

where $\gamma \in \mathbb{R}^+, b \in \mathbb{R}, w \in \mathbb{R}^h$. Thanks to the first regularization term in the objective function, the complexity of the model is controlled and therefore overfitting problem is avoided [22]. In the LS-SVM approach the feature map φ is not explicitly known in general and can be infinite dimensional. Therefore the kernel trick is used and the problem is solved in the dual [22]. The Lagrangian of the constrained optimization problem (2) becomes:

$$
\mathcal{L}(w, b, e_i, \alpha_i) = \frac{1}{2}\, w^T w + \frac{\gamma}{2} e^T e - \sum_{i=1}^{N} \alpha_i \Big[w^T \varphi(t_i) + b + e_i - y_i \Big] \tag{3}
$$

where $\{\alpha_i\}_{i=1}^N$ are Lagrange multipliers. Then the Karush-Kuhn-Tucker (KKT) optimality conditions are as follows,

$$
\begin{aligned}
&\frac{\partial \mathcal{L}}{\partial w} = 0 \rightarrow w = \sum_{i=1}^{N} \alpha_i \varphi(t_i), \\
&\frac{\partial \mathcal{L}}{\partial e_i} = 0 \rightarrow \alpha_i = \gamma e_i, \\
&\frac{\partial \mathcal{L}}{\partial b} = 0 \rightarrow \sum_{i=1}^{N} \alpha_i = 0, \\
&\frac{\partial \mathcal{L}}{\partial \alpha_i} = 0 \rightarrow w^T \varphi(t_i) + b + e_i = y_i.
\end{aligned} \tag{4}
$$

Eliminating the primal variables e_i and w leads to the following linear system in the dual problem:

$$
\left[\begin{array}{c|c} \Omega + I_N/\gamma & 1_N \\ \hline 1_N^T & 0 \end{array} \right] \left[\begin{array}{c} \alpha \\ \hline b \end{array} \right] = \left[\begin{array}{c} y \\ \hline 0 \end{array} \right] \tag{5}
$$

where $\Omega_{ij} = K(t_i, t_j) = \varphi(t_i)^T \varphi(t_j)$ is the ij-th entry of the positive definite kernel matrix. $1_N = [1, \ldots, 1]^T \in \mathbb{R}^N$, $\alpha = [\alpha_1, \ldots, \alpha_N]^T$, $y = [y_1, \ldots, y_N]^T$ and I_N is the identity matrix. The model in the dual form becomes:

$$
y(t) = w^T \varphi(t) + b = \sum_{i=1}^{N} \alpha_i K(t, t_i) + b. \tag{6}
$$

3. Time Delay Estimation in a System with Input Delay

3.1. Problem Statement

Systems with input delays are ubiquitous and widely used in modelling of real phenomena such as in control theory, population dynamics [11] and engine cooling systems [5]. The delay can be constant, time varying or state dependent. For instance in milling processes, speed-dependent delays arise due to the deformation of the cutting tool [1].

A typical first order single input delay model may be expressed as:

$$
\dot{x}(t) = f(t, x(t), u(t - \theta), p(t)), \quad t \geq t_0, \tag{7}
$$

where $p(t)$ is the parameter vector, u is the input to the system and θ is the time delay or lag which is nonnegative and can be either constant or depend on time or state, that is, $\theta = \theta(t, x(t))$. The initial time is denoted by t_0.

The determination of these unknown time delay parameters have been considered by many different authors (see, for example [2, 3, 6]). The majority of the proposed approaches first simulate the dynamic system using some initial guess for the parameters. Next, the model predictions are compared with the measured data and updated using some optimization algorithm. Such methods are computationally expensive as they require multiple integrations of the process in order to obtain a final parameter estimate.

Mehrkanoon *et al.* [15, 13] proposed an approach based on least squares support vector machines for constant and time-varying parameter estimation of dynamical systems governed by ordinary differential equations. The proposed method allowed for the development of an integration-free, LS-SVM-based approach for the estimation of the unknown time delay parameter and the history function in delay differential equation (systems with state-delay) [14]. In this proposed approach, the estimation of the time delay parameter is converted into an algebraic optimization problem.

For the purposes of this paper, it will be assumed that the original nonlinear Equation (7) can be written in a parameter-affine form as

$$\dot{x}(t) = f(t, x(t), p)u(t-\theta), \quad t \geq t_0, \tag{8}$$

where $f(\cdot) : \mathbb{R}^3 \to \mathbb{R}$ is an arbitrary nonlinear function and θ is the constant time delay parameter of the system. If the system is not parameter affine, the approach still would be possible but then one has to solve a non-convex optimization to get an estimate of the unknown time delay parameter. In the proposed method, the objective is to estimate θ given that p could also be unknown. The state of the system is measured that is

$$y(t_i) = x(t_i) + e(t_i), i = 1, ..., N, \tag{9}$$

where $\{e(t_i)\}_{i=1}^N$ are independent measurement errors with zero mean.

3.2. Methodology

The method proposed by [14] will be used to estimate the unknown parameters of the system for both closed- and open-loop process conditions. The method consists of two steps. In the first step, a kernel-based model, LS-SVM, is used to obtain a closed-form expressions for the state and its derivative, $\frac{d}{dt}\hat{x}(t)$ and $\hat{x}(t)$. Given the observational data, the LS-SVM formulation (2) approximates the state of the system and has the following form in the dual:

$$\hat{x}(t) = w^T\varphi(t) + b = \sum_{i=1}^N \alpha_i K(t_i, t) + b, \tag{10}$$

where K is the kernel function. Making use of Mercer's theorem [23], derivatives of the feature map $\varphi(\cdot)$, can be written in terms of derivatives of the kernel function. Therefore, one can obtain a closed-form approximate expression for the derivative of the model (15) with respect to time: [16, 12],

$$\frac{d}{dt}\hat{x}(t) = w^T\dot{\varphi}(t) = \sum_{i=1}^N \alpha_i K_s(t_i, t), \tag{11}$$

where $K_s(t, s) = \frac{\partial(\varphi(t)^T\varphi(s))}{\partial s}$.

In the second step, the explicit LS-SVM model

$$\hat{u}_\theta(t) = v^T\psi(t) + d, \tag{12}$$

is assumed as an approximation for the term $u(t-\theta)$ where $\psi(\cdot) : \mathbb{R} \to \mathbb{R}^{\tilde{h}}$ is the feature map.

Substituting the closed-form expressions for the state and its derivative, $\frac{d}{dt}\hat{x}(t)$ and $\hat{x}(t)$ obtained from Equations (15) and (11) respectively, into the model description given by Equation (8), the unknown parameters v and d are identified as those minimizing the following optimization problem:

$$\begin{aligned} \underset{v,d,e}{\text{minimize}} \quad & \frac{1}{2}v^Tv + \frac{\gamma}{2}\sum_{i=1}^N e_i^2 \\ \text{subject to} \quad & \frac{d}{dt}\hat{x}(t_i) = f(t_i, \hat{x}(t_i), p)\left(v^T\psi(t_i) + d\right) + e_i, \ i = 1, ..., N. \end{aligned} \tag{13}$$

Lemma 3.1. *Given a positive definite kernel function $\tilde{K} : \mathbb{R} \times \mathbb{R} \to \mathbb{R}$ with $\tilde{K}(t,s) = \psi(t)^T\psi(s)$ and a regularization constant $\gamma \in \mathbb{R}^+$, the solution to Equation (13) is given by the following dual problem*

$$\left[\begin{array}{c|c} D\tilde{\Omega}D + \gamma^{-1}I & F \\ \hline F^T & 0 \end{array}\right]\left[\begin{array}{c} \tilde{\alpha} \\ \hline d \end{array}\right] = \left[\begin{array}{c} \frac{d\hat{x}}{dt} \\ \hline 0 \end{array}\right] \tag{14}$$

where $\tilde{\Omega}_{i,j} = \tilde{K}(t_i, t_j) = \psi(t_i)^T\psi(t_j)$ is the (i, j)-th entry of the positive definite kernel matrix and I is the identity matrix. Furthermore, $\tilde{\alpha} = [\tilde{\alpha}_1, \ldots, \tilde{\alpha}_N]^T$, $F = [f(t_1, \hat{x}(t_1), p), \ldots, f(t_N, \hat{x}(t_N), p)]^T$, $\frac{d\hat{x}}{dt} = [\frac{d}{dt}\hat{x}(t_1), \ldots, \frac{d}{dt}\hat{x}(t_N)]^T$. D is a diagonal matrix with the elements of F on the main diagonal. Moreover, the model in dual form becomes

$$\hat{u}_\theta(t) = v^T\psi(t) + d = \sum_{i=1}^{N} \tilde{\alpha}_i \tilde{K}(t_i, t) + d, \tag{15}$$

Proof 3.1. Similar to the proof given in [14], we start with constructing the Lagrangian, deriving the KKT optimality conditions and finally eliminating the primal variables. The Lagrangian of the constrained optimization problem (13) becomes

$$\begin{aligned} \mathcal{L}(v, d, e_i, \alpha_i) = \frac{1}{2} v^T v + \frac{\gamma}{2} \sum_{i=1}^{M} e_i^2 - \sum_{i=1}^{M} \tilde{\alpha}_i \Big[\Big(v^T\psi(t_i) + d\Big) f(t_i, \hat{x}(t_i), p) \\ + e_i - \frac{d}{dt}\hat{x}(t_i)\Big], \end{aligned} \tag{16}$$

where $\{\alpha_i\}_{i=1}^M$ are Lagrange multipliers. Then the Karush-Kuhn-Tucker (KKT) optimality conditions are as follows,

$$\begin{aligned} &\frac{\partial \mathcal{L}}{\partial v} = 0 \to\ v = \sum_{i=1}^{N} \tilde{\alpha}_i f(t_i, \hat{x}(t_i), p)\psi(t_i), \\ &\frac{\partial \mathcal{L}}{\partial d} = 0 \to\ \sum_{i=1}^{N} \tilde{\alpha}_i f(t_i, \hat{x}(t_i), p) = 0, \\ &\frac{\partial \mathcal{L}}{\partial e_i} = 0 \to\ e_i = \frac{\tilde{\alpha}_i}{\gamma},\ \ i = 1, \ldots, N, \\ &\frac{\partial \mathcal{L}}{\partial \alpha_i} = 0 \to\ \Big(v^T\psi(t_i) + d\Big) f(t_i, \hat{x}(t_i), p) + e_i = \frac{d}{dt}\hat{x}(t_i),\ \ i = 1, \ldots, N. \end{aligned} \tag{17}$$

After elimination of the primal variables v and $\{e_i\}_{i=1}^M$ and applying Mercer's Theorem yields the linear system in (14). □

After obtaining an approximate $\hat{u}_\theta(t)$ for the delay term, the cross-correlation method described in [14] is used to estimate the fixed time delay θ. The process of estimating the unknown delay τ is described in Algorithm 1.

4. Process Model and Description

4.1. Background

In order to examine and understand the properties of the proposed time delay estimation method, a series of simulations and experiments will be performed on a continuous, stirred, heated tank (CSHT). Theoretical models of the system with parameter values based on the experimental system will be used to perform the simulations. A schematic of the experimental system is shown in Figure 1. The salient features of this system are:

1. The level in the tank is controlled by the cold water flow rate. In practice, the controller is sufficiently fast and good that the level in the tank during the course of an experiment will stay constant and deviate by less than 1 mm.

Algorithm 1: Approximating the constant time delay parameter for System (8)

Input: The external input $u(t)$, the measured output $y(t)$, sampling time t_s, and a physical model describing the system

Output: An estimate for the time delay parameter, θ

First Stage: Estimating the State Trajectory and its Derivative

Approximate the state trajectories $x(t)$ based on the LS-SVM model (see Eq. (15)).

Approximate the state derivative using Eq. (11).

Second Stage: Estimating the Time Delay Parameter

Estimate the delay term $u(t+\theta)$ by solving the optimization problem (13).

Estimate the time delay parameter θ using available information about $u(t)$ and $u(t+\theta)$ estimation by means of cross-correlation [14].

2. The temperature in the tank is controlled by the steam flow rate. Due to the significant time delay present in the system, the control is weaker and slower. Furthermore, fluctuations in the cold water temperature have an appreciably effect on the overall system behaviour.
3. The flow out of the tank is controlled by a manual hand valve. Changing the hand valve position will change the characteristics of the system.

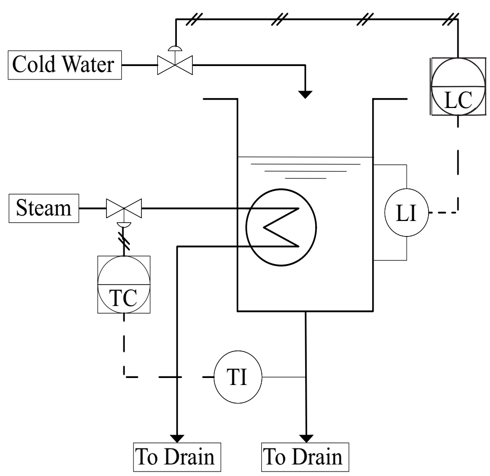


Figure 1: Schematic of the continuous, stirred, heated tank

4.2. Theoretical Process Model

The theoretical models of the system can be developed by writing mass and energy balances for the system at hand. Since it has been assumed that the level in the tank is more or less constant and does not need to be considered, the mass balance will likewise not be considered. The derivation is based on [18]. For a general system, the energy balance can be written as

$$\frac{dE}{dt} = \dot{E}_{in} - \dot{E}_{out} \tag{18}$$

where E is the energy in the tank and $\dot{E}$ is the energy flow. The energy in the tank can be rewritten as

$$E = mc_p\left(T - T_{ref}\right) = \rho A h c_p\left(T - T_{ref}\right) \tag{19}$$

where ρ is the density, A the cross-sectional area of the tank, h the height in the tank, m the mass of water in the tank, c_p the heat capacity, T the temperature, and T_{ref} an arbitrary reference temperature. In a similar manner, the energy flow in and out of the tank can be written as:

$$\dot{E}_{cold_{in}} = \dot{m}_{in} c_p \left(T_{in} - T_{ref}\right) \tag{20}$$

$$\dot{E}_{cold_{out}} = \dot{m}_{out} c_p \left(T_{out} - T_{ref}\right) = R\sqrt{h} c_p \left(T_{out} - T_{ref}\right) \tag{21}$$

where $\dot{m}_{in}$ is the inlet flow rate, T_{in} the temperature of the cold water stream, $\dot{m}_{in}$ he outlet flow rate, T_{out} the outlet temperature, and R the resistance constant for flow out of an orifice. It can be noted that the flow out of the tank has been assumed to be gravity-driven, Bernoulli flow. Finally, the energy flow into the system due to the condensation of the steam can be written as

$$\dot{E}_{steam} = \dot{m}_{steam}\left(t - \theta\right) F \Delta H \tag{22}$$

where F is the fraction of steam condensed, θ the time delay, and ΔH the enthalpy of condensation for saturated steam at 150 psig. Combining the simplifications given as Equations (19), (20), (21), (22) into Equation (18) gives

$$\begin{aligned} &\rho A c_p \frac{dh\left(T - T_{ref}\right)}{dt} = \\ &\dot{m}_{in} c_p \left(T_{in} - T_{ref}\right) + \dot{m}_{steam}\left(t - \theta\right) F \Delta H - R\sqrt{h} c_p \left(T_{out} - T_{ref}\right) \end{aligned} \tag{23}$$

Simplifying Equation (23) and taking into consideration the previously made assumptions about the system gives the overall energy balance for the system as

$$\frac{dT}{dt} = \frac{\dot{m}_{in}}{\rho A h}\left(T_{in} - T\right) + \dot{m}_{steam}\left(t - \theta\right) \frac{F \Delta H}{\rho A h c_p} \tag{24}$$

It can be noted that this equation is an affine linear differential equation of the form (8) where u is $\dot{m}_{steam}$, T is the state of the system and T_{in} is part of the model parameters (p in equation (8)) that need be estimated. If it is assumed that T_{in} does not vary within the time frame considered, then Equation (24) reduces to a standard, first-order differential equation. Furthermore, it can be noted that F can be computed for a system using available steady-state values.

4.3. Model Parameters

In order to obtain parameter values for the simulation, multiple step tests were performed on the pilot scale system for different conditions and situations in order to obtain a representative sample of the operating conditions. It was observed that the cold water temperature had a significant impact on the overall process characteristics, but it did not affect the measured time delay. The cold water temperature varied between 4°C to 20°C. However, assuming that the conditions remain the same, the parameter estimates are reproducible. Typical steady-state parameter values for the single, heated tank system are provided in Table 1.

These values compare well with the values obtained from performing system identification on the heated tank. In simulations, these values will be used to obtain the data on which the time delay estimation method will be considered. Similarly, these values will form the benchmark against which the identified system parameters can be compared.

5. Simulated CSHT Example

For the simulations, the model given by Equation 24 will be used to examine the theoretical performance of the system for 3 different cases: slowly varying inlet temperature, pseudorandom binary input signal (prbs), and random sampling of output for different operating conditions. As well, the routine operating data case will be considered All parameter values are based on the values presented in Table 1. It should be noted that all of these cases considered in this simulation case cannot be solved using the standard time delay identification methods.

Table 1: Parameter values for the experiment

Parameter	Value	Parameter	Value
h_{ss}(m)	0.20	T_{ss}(°C)	24
$\rho(kg \cdot m^{-3})$	1000	$\dot{m}_{\text{in}}$ (kg/min)	6
c_p(kJ·kg^{-1}·K^{-1})	4.186	$\dot{m}_{\text{steam}}$ (kg/min)	15
ΔH (kJ/kg) (at 1,035 kPa)	2100	D_T (m)	0.18
T_{in}(°C)	4	T_{ref}(°C)	0
Hand Valve (°)	45	θ (s)	40
R(kg·min^{-1}·m$^{-0.5}$)	13.42	F	0.957

5.1. Case I: Slowly Varying Inlet Temperature

The first case will consider the situation where the inlet temperature is slowly varying during the course of the experiment. Both the open- and closed-loop cases will be considered. A step change in the input (or reference) signals will be made.

Additional information will be obtained by taking the data from a single simulation and adding different levels of measurement noise to the output to examine the impact of the signal-to-noise ratio (SNR) to the estimation of the parameters. The search region for the inlet water temperature, T_{in}, was defined as [4, 20]. In order to investigate the impact of the unmeasured cold water temperature on time delay estimation, the inlet water temperature region was partitioned into 10 equal regions. For each region, an estimate of the time delay was obtained and the evolution of the system with respect to time plotted. This procedure was repeated for four different signal-to-noise ratios: 56.2205, 43.7422, 40.1927, and 37.817.

Figure 2 shows the temperature plot as a function of time. It should be noted that although the true inlet temperature is slowly varying, it was assumed for the purposes of this simulation to assume that the inlet temperature was constant at 10°C. It can be seen that the match between the estimated and measured temperature values is very close. Furthermore, Figure 3 shows the measured and estimated steam flow rates. The estimated steam value is back calculated from the predicted temperature values in order to eliminate the time delay. The time delay is then estimated using the cross-correlation between the estimated and measured steam values. As shown in Figure 4 the estimated time delay is assumed to correspond to the lag which produces the largest cross-correlation value. Again, a value of approximately 40 s is suggested as being the optimal time delay estimate.

Table 2 presents the mean and standard deviation of the estimated time delays as a function of the signal-to-noise ratio and the inlet temperature for 10 simulations. It can be seen that the smaller the signal-to-noise ratio the larger the variability in the time delays estimated. In all cases, the true value of 40 s is covered by the 95% confidence intervals for the given parameters. Thus, since all of the methods obtain a time delay estimate close to the one, it can be concluded that the approach can indeed recover the true time delay.

Therefore, the above results suggest that for the case of a slowly-varying, unmeasured time inlet temperature, it is possible to use this method to estimate the time delay. Furthermore, the impact of noise is minimal on the overall estimate of the time delay.

Table 2: Case I: Mean Values and Standard Deviations for 10 Simulations with Different Noise and Assumed Inlet Temperature (T_{in}) for Estimating the Time Delay using slowly-varying inlet temperature data

	Inlet Temperature, $T_{in}(°C)$				
SNR	4.00	8.00	12.00	16.00	20.00
56.220491	41.0 ± 0.00	41.0 ± 0.00	41.3 ± 0.58	41.3 ± 0.58	41.0 ± 0.00
43.742161	40.0 ± 1.00	40.3 ± 2.31	40.0 ± 1.00	40.7 ± 2.31	41.7 ± 0.58
40.192684	40.7 ± 0.58	40.0 ± 2.65	38.7 ± 2.52	41.3 ± 0.58	38.7 ± 0.58
37.817817	39.3 ± 5.03	39.3 ± 3.51	41.0 ± 5.20	44.0 ± 3.46	42.0 ± 1.73

The results for the case where the data is taken from a system running in closed loop is very similar to the open-loop results. For this reason, the results are not shown in detail here.

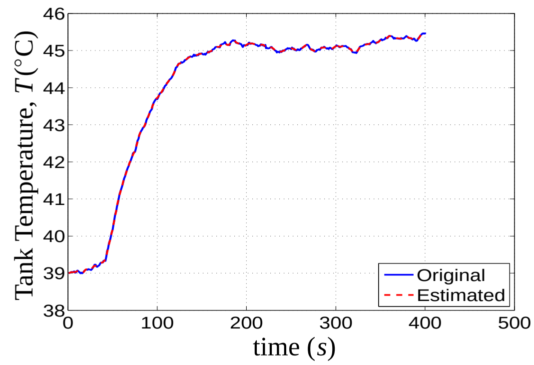


Figure 2: Case I: Open-Loop Estimation of the Tank Temperature T for the slowly-varying inlet temperature case

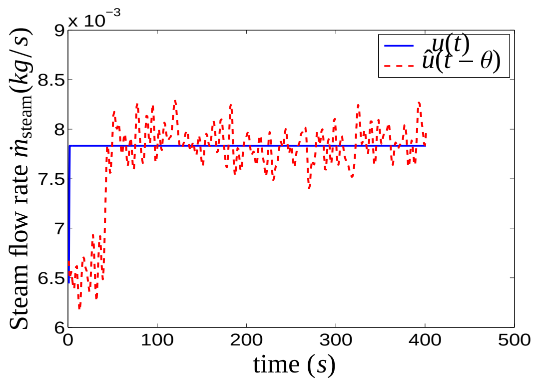


Figure 3: Case I: Time Delay Estimation with Slowly-Varying Inlet Temperature: Estimation of the steam flow rate $\dot{m}_{\text{steam}}$ when T_{in} equals 10°C.

5.2. Case II: Pseudorandom Binary Signal

Although step tests are commonly used in industrial applications, in many identification experiments, even on industrial systems, pseudorandom binary signals (prbs) are used instead. Such signals have the advantage that they approximate white noise with only two levels. However, using pseudorandom binary signals implies that many of the commonly used methods for time delay estimation cannot be used, since they require step test behaviour or true white noise inputs. Using the same situation as for case I, including a slowly varying inlet temperature, the results for closed-loop behaviour are examined. The open-loop results are very similar to the closed-loop results. A simple proportional and integral (PI) controller is used to control the system. All changes are made to the reference signal to the process.

Figure 5 compares the predicted and measured process evolution. The layout and interpretation of the figures and table is the same as for case I above. As before, Figure 5(a) shows that the match between the estimated and measured temperature values is very close. From Figure 5(b), which shows that the measured and time-delayed, estimated steam flow rates, is approximately 40 s. Finally, Figure 5(c) shows that the inlet temperature does not affect the estimation of the time delay with an optimal value being 40 s.

Table 3 shows the estimated time delays as a function of SNR and assumed T_{in} for 10 simulations. Once again, the assumed inlet temperature does not influence the estimated time delay significantly. On the other hand, for small SNR values, the ability of the system to accurately determine the time delay is diminished. It can be noted that the result is that there are now a much larger variance of the values and extreme value more strongly impact the overall results. Except for this difference, the overall results are very similar to those previously obtained.

Thus, this suggests that the proposed method, unlike some of the commonly used methods, can indeed be used for time delay estimation, even if the input signal is a pseudorandom binary signal.

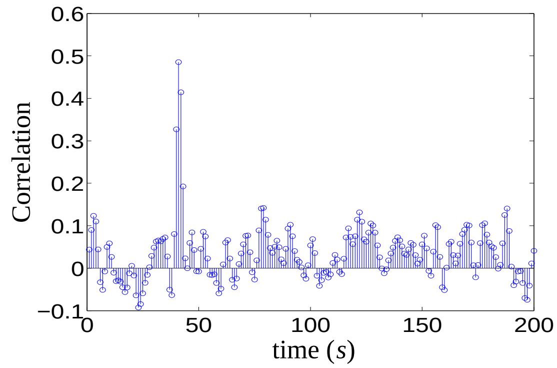


Figure 4: Case I: Time Delay Estimation with Slowly-Varying Inlet Temperature: The cross-correlation between $u(t)$ and $\hat{u}(t-\theta)$.

Table 3: Case II: Time Delay Estimation with a PRB Signal and a Slowly-Varying Inlet Temperature: Mean Values and Standard Deviations for 10 simulations with different noise and assumed inlet temperature (T_{in})

	Inlet Temperature, $T_{in}(^{\circ}C)$				
SNR	4.00	8.00	12.00	16.00	20.00
71.05	40.1 ± 0.32	40.0 ± 0.00	40.4 ± 0.52	40.1 ± 0.32	40.4 ± 0.52
59.16	41.0 ± 0.00	41.0 ± 0.00	41.0 ± 0.00	40.9 ± 0.32	40.9 ± 0.32
55.37	41.0 ± 0.00	41.0 ± 0.00	41.0 ± 0.47	41.1 ± 0.32	41.0 ± 0.00
52.94	41.2 ± 0.42	41.2 ± 0.63	74.4 ± 104.92	107.6 ± 140.41	76.7 ± 112.54

5.3. *Case III: Random Sampling of Output*

The third case will consider the situation where the sampling rate of the output temperature is not constant. Industrially, this could be observed if the communication set up losses data packets and not all of the available information that has been measured is recorded for subsequent retrieval. For the purposes of this experiment, it will be assumed that the dropping is random, but is not greater than 15%. Finally, it will be assumed that the inlet temperature is constant.

Figure 6 compares the predicted and measured process evolution. The layout and interpretation of the figures are the same as for the previous case above. As before, Figure 6(a) shows that the match between the estimated and measured temperature values is very close. From Figure 6(b), shows that the estimated steam flow rate is now much more variable compared with the original more or less flat steam flow rate. This jaggedness is partly a result of the random sampling of the signal.

Table 4 presents the estimated time delays as a function of the signal-to-noise ratio and the assumed inlet temperature. Once again, the inlet temperature does not influence the estimated time delay significantly nor does the signal-to-noise ratio. It is interesting to note that here that estimated time delays are uniformly less than the expected value of 40 s. In fact, even if the confidence intervals are constructed for these examples, few of them will cover or come close to the true value. This discrepancy can be attributed to the loss of information created by the randomness of the signal. Nevertheless, this method is better than the other methods as it can natively handle a randomly sampled signal.

Table 4: Case III: Random Sampling of Temperature Signal: Mean Values and Standard Deviations for 10 Simulations with Different Noise and Inlet Temperature (T_{in})

	Inlet Temperature, $T_{in}(^{\circ}C)$				
SNR	4.00	8.00	12.00	16.00	20.00
57.34	37.2 ± 0.63	37.0 ± 0.47	37.5 ± 0.71	37.1 ± 0.57	37.5 ± 0.97
45.14	35.8 ± 1.93	35.6 ± 1.26	34.7 ± 0.95	35.7 ± 1.89	35.3 ± 1.70
41.56	34.2 ± 1.62	33.1 ± 2.02	33.8 ± 2.39	33.9 ± 2.92	33.3 ± 2.06
39.29	33.5 ± 2.01	32.8 ± 2.35	33.7 ± 2.87	32.5 ± 2.12	32.3 ± 2.75

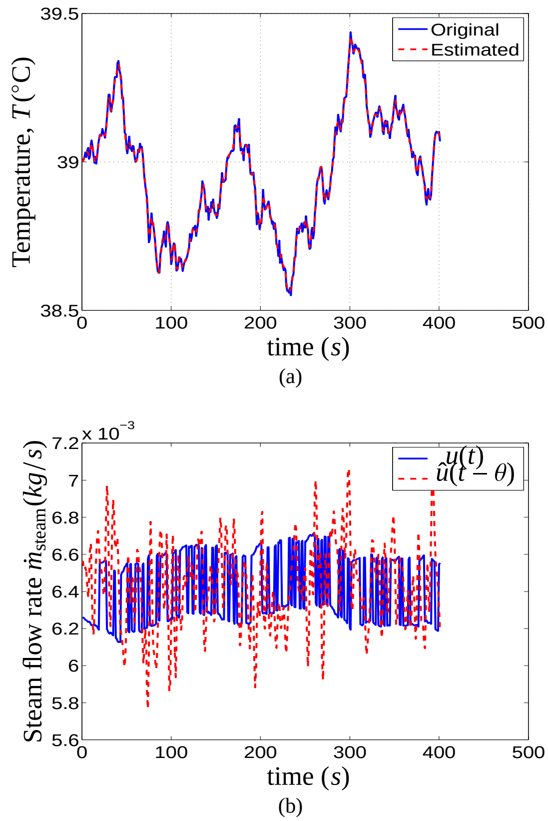


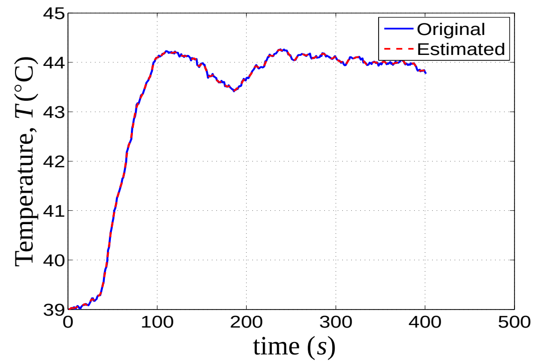
Figure 5: Case II: Time Delay Estimation with a PRB Signal and a Slowly-Varying Inlet Temperature: (a) Temperature Estimation and (b) Steam Flow Rate Estimation

5.4. Case IV: Routine Operating Data

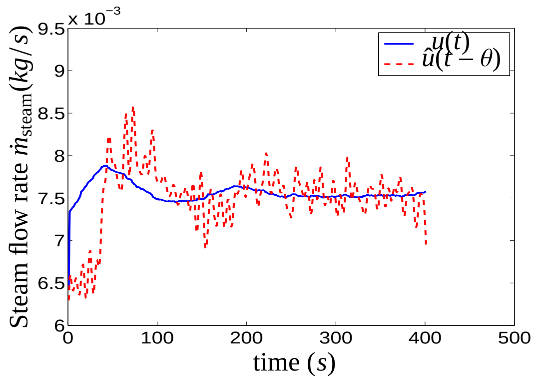
The fourth, and final, case will consider the situation where a process is being run with a controller and the reference signal is not changing its value, that is, the data set is said to be routine operating data. A simple proportional and integral (PI) controller was used to control the system, so as to minimize oscillations and increase speed of response. Figure 7 compares the predicted and measured process evolution, while Table 5 shows the estimated time delays as a function of SNR and T_{in}. The layout and interpretation of the figures and table is the same as for the cases above. As before, Figure 7(a) shows that the match between the estimated and measured temperature values is very close. From Figure 7(b), which shows that the measured and time-delayed, estimated steam flow rates, is approximately 40 s. Finally, Figure 7(c) shows that the inlet temperature does not affect the estimation of the time delay with an optimal value being 40 s.

Table 5 presents the estimated time delays as a function of the signal-to-noise ratio and the inlet temperature. Once again, the inlet temperature does not influence the estimated time delay significantly nor does the signal-to-noise ratio. In fact, the values cluster around 40 s, which is the true time delay for the simulation system. It is interesting to note that the standard deviation has decreased in this case.

Thus, the above results suggest that for a closed-loop process without reference signal excitation, it is possible to use this method to estimate the time delay, even if some of the parameter are not measured. Furthermore, the impact of noise is minimal on the overall estimate of the time delay. This result has the potential implication that it could be possible to relatively easily estimate the time delay for an unknown process for use with a control performance assessment measure, such as the Harris Index [19]. This means that it will not now be necessarily to know the process time delay in order to apply this method.



(a)

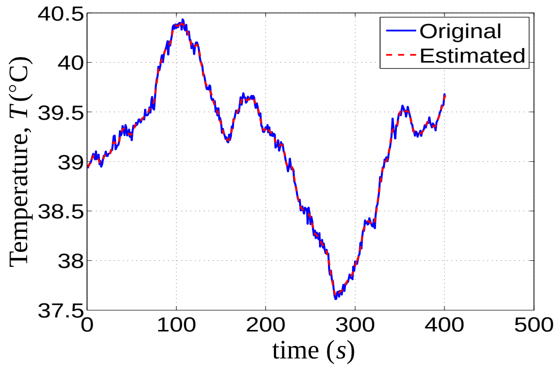


(b)

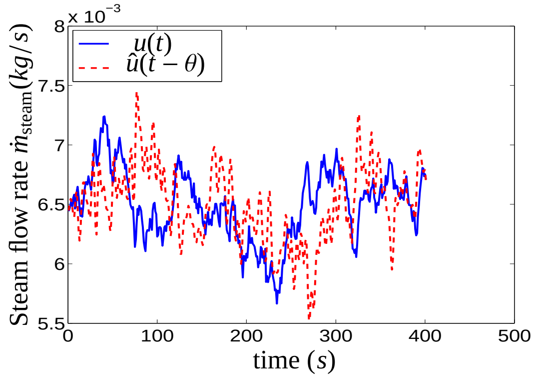
Figure 6: Case III: Random Sampling of Temperature Signal: (a) Temperature Estimation and (b) Steam Flow Rate Estimation

Table 5: Case IV: Estimating Time Delay Using Routine Operating Data: Mean Values and Standard Deviations for 10 Simulations with Different Noise and Assumed Inlet Temperature (T_{in})

	Inlet Temperature, $T_{in}(°C)$									
SNR	4.00	5.77	7.55	9.33	11.11	12.88	14.66	16.44	18.22	20
61.64	39.60 ± 0.54	39.60 ± 0.52	38.80 ± 0.44	39.80 ± 0.44	40.00 ± 0.00	39.60 ± 0.54	39.60 ± 0.54	39.80 ± 0.44	39.60 ± 0.54	39.40 ± 0.54
49.58	40.00 ± 0.70	39.80 ± 0.83	39.80 ± 0.83	40.00 ± 0.70	40.20 ± 0.83	39.40 ± 0.54	40.40 ± 0.89	40.00 ± 0.10	40.20 ± 0.83	39.60 ± 1.14
45.58	40.60 ± 0.54	40.00 ± 1.00	40.20 ± 1.09	40.20 ± 1.78	40.80 ± 1.30	40.40 ± 1.51	40.40 ± 1.14	40.40 ± 0.54	40.00 ± 1.22	40.80 ± 0.83
43.24	41.00 ± 0.70	40.60 ± 0.89	40.20 ± 0.44	41.20 ± 1.30	40.00 ± 1.73	40.40 ± 1.14	40.80 ± 1.48	40.80 ± 0.44	41.60 ± 0.70	40.80 ± 0.83



(a)



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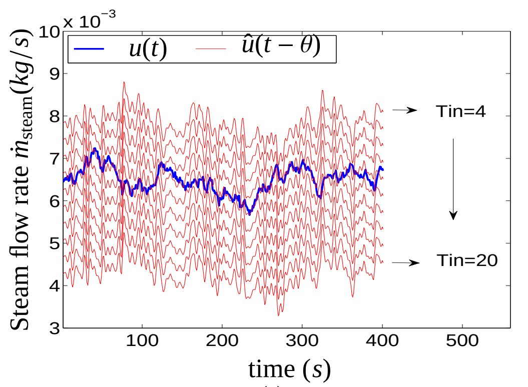

(c)

Figure 7: Case IV: Estimating Time Delay Using Routine Operating Data: (a) Estimation of the Temperature T. (b) Estimation of the steam flow rate $\dot{m}_{\text{steam}}$ when T_{in} is set to 10. (c) Estimation of the steam flow rate $\dot{m}_{\text{steam}}$ when T_{in} is varying in the range $[4, 20]$.

5.5. *Comparison of the Proposed Time Delay Estimation Method with Other Such Methods for the Simulation Data*

This section will compare the proposed method with other available methods for estimating the time delay, including the Laguerre method described in [4], as an example of the implicit method for estimating the time delay; the ARMAX-based method implemented by MATLAB's DELAYEST function, as an example of the explicit method for estimating the time delay; and the cross-correlation method, as an example of the area and moment approach to estimating the time delay.

Table 6 summarises the results for the different cases. Firstly, it can be noted that only the ARMAX-based method can be used for all cases, while the cross-correlation method only provides accurate estimates when the input is approximately a white noise signal. Secondly, it can be seen that the ARMAX-based method provides time delay estimates that are strongly dependent both on the orders selected for testing and the individual circumstances. For example, for case I, the ARMAX-based method cannot provide a reasonable time delay estimate. On the other hand, the estimates provided by the proposed time delay method can accurately estimate the time delay irrespective of the underlying conditions. Furthermore, even in the case where there is missing information, the proposed method can provide a reasonable, if not necessarily completely correct, estimate of the time delay. This shows that the proposed method can be applied to a wide range of different situations, which often cannot be solved by conventional methods.

Table 6: Comparing the Performance of the Proposed Method, the Cross-Correlation Method (CRA), the ARMAX-based method implemented by MATLAB's DELAYEST, and the Laguerre Methods for Estimating the Time Delay Using Simulation Data

	Method					
	CRA	DELAYEST		Laguerre Method	Proposed	True value
Data Set		Model Order = 1	Model Order = 10			
Case I: Open-Loop	N.A.	2	15	52.4	40	40
Case I: Closed-Loop	N.A.	47	98	52.4	40	40
Case II: Open-Loop	40	41	40	39.6	40	40
Case II: Closed-Loop	41.	41	40	43.1	40	40
Case III	N.A.	N.A.	N.A.	N.A.	35	40
Case IV	41	41	39	50.1	40	40

6. Experimental CSHT Example

Having considered some complex cases in the simulation examples, a series of experiments on a pilot scale heated tank system will now be performed to examine the impact that an actual system has on the method. It should be noted that the data sets were extracted from a data historian and hence were not performed specifically for this experiment. Such a task is very common when trying to obtain models for industrial systems, especially when designing soft sensors. Extracting useful information from historical data sets forms one area of data mining.

The experimental system has nominal parameters similar to those shown in Table 1. Due to fluctuations in the system parameters as well as unexpected disturbances, the process values can change slightly over the course of the experiment. As before, 3 different cases will be consider: open loop, closed loop with external excitation, and routine operating data.

6.1. *Experimental Validation of the Time Delay Estimation Algorithm using Open-Loop Data*

The first case will examine the application of this method to open-loop experimental data. For estimating the time delay using an open-loop, the only available situation was when a single step test was performed and the system allowed to reach steady state. In this case, a simple step change of 5 kg/h was performed in the steam flow rate and the system was allowed to reach steady state. It should be noted that step tests are commonly used in industry to determine simple process models [17].

Figures 8(a) and (b) show the estimated and observed temperature and steam flow rate as a function of time. Once again, it should be noted that the estimated steam flow rates are shifted by the time delay, since they are computed assuming no time delay from the measured temperature values. Visually, based on the difference between the observed and estimated steam flow rates, it would seem that the time delay is about 40 s. It can also be noted that the assumed inlet temperature of 10°C is probably too high, since the graphs do not match very well. However, this should not be too much of an issue, as the simulations have shown that the precise value of the inlet temperature is not required.

Figure 8(c) shows the predicted steam flow rate for different T_{in} values. As before, it is quite clear that the specific cold water inlet temperature does not have an impact on the overall ability to estimate the time delay. It would seem that the cold water inlet temperature is closer to 4°C, then the assumed value of 10°C. This is a plausible result since the run occurred on a cold winter's day in February. The utility water would then be close to its lower value.

Finally, Figure 8(d) shows the estimated time delay θ as a function of T_{in}, along with the standard deviation obtained for 10 simulation runs. It can be seen that the effect of T_{in} is minimal on the overall estimation of the time delay. The values range from 42.8 s at 4°C to 42.60 s at 20°C. It can be noted that the tight bounds and small over all range strongly confirm that an additive disturbance does not influence the estimation of the time delay.

6.2. Experimental Validation of Time Delay Estimation Method using Closed-Loop Process Data with Reference Signal Excitation

The second case will consider the application of this method to closed-loop process data where there has been a change in the reference signal. The same system and physical parameters will be used as for the open-loop case. A simple PI-controller was used to close the loop. A step change of 5°C in the setpoint was made. This change in the setpoint provides external excitation for the process.

Figures 9(a) and (b) show the estimated and observed temperature and steam flow rate as a function of time. Once again, it should be noted that the estimated steam flow rates are shifted by the time delay, since they are computed assuming no time delay from the measured temperature values. Visually, based on the difference between the observed and estimated steam flow rates, it would seem that the time delay is about 40 s.

Figure 9(c) shows the predicted steam flow rate for different T_{in} values. As before, it is quite clear that the specific cold water inlet temperature does not have an impact on the overall ability to estimate the time delay. It would seem that the cold water inlet temperature is closer to 4°C, then the assumed value of 10°C. This is a plausible result since the run occurred on a cold winter's day in February. The utility water would then be close to its lower value.

Finally, Figure 9(d) shows the estimated time delay θ as a function of T_{in}, along with the standard deviation obtained for 10 simulation runs. It can be seen that the effect of T_{in} is minimal on the overall estimation of the time delay. The values range from 47.7 s at 4°C to 45.9 s at 20°C. The error bars decrease as the inlet temperature increases. It can be noted that the tight bounds and small over all range strongly confirm that an additive disturbance does not influence the estimation of the time delay.

6.3. Experimental Validation of the Time Delay Estimation using Routine Operating Data

The third and final case will consider the application of the method to routine operating data. The same system and physical parameters will be used as for the previous closed-loop case. The system was run at a constant reference signal through the experiment. This implies that there is no excitation coming to the process from the reference signal. The only source of excitation is caused by disturbances, such as the cold water inlet temperature.

Figures 10(a) and (b) show the estimated and observed temperature and steam flow rate as a function of time. Once again, it should be noted that the estimated steam flow rates are shifted by the time delay, since they are computed assuming no time delay from the measured temperature values. Visually, based on the difference between the observed and estimated steam flow rates, it would seem that the time delay is about 40 s.

Figure 10(c) shows the predicted steam flow rate for different T_{in} values. As before, it is quite clear that the specific cold water inlet temperature does not have an impact on the overall ability to estimate the time delay. It would seem that the cold water inlet temperature is closer to 20°C, then the assumed value of 10°C. Although this may seem quite odd in comparison with the previous 2 cases, it should be noted that the routine operating data was extracted under different ambient conditions, namely that of summer, and additional stress was placed on the utility stream, so that the water temperature upon arrival in the experimental set up had significantly increased. Unfortunately, the inability to measure this temperature meant that the exact values are not known and the causes must be ascribed based on experience with the system [18].

Finally, Figure 10(d) shows the estimated time delay θ as a function of T_{in}, along with the standard deviation obtained for 10 simulation runs. It can be seen that the effect of T_{in} is minimal on the overall estimation of the time delay. The values range from 38.0 s at 4°C to 38.5 s at 20°C. The error bars decrease as the inlet temperature increases. It can be noted that the tight bounds and small over all range strongly confirm that an additive disturbance does not influence the estimation of the time delay.

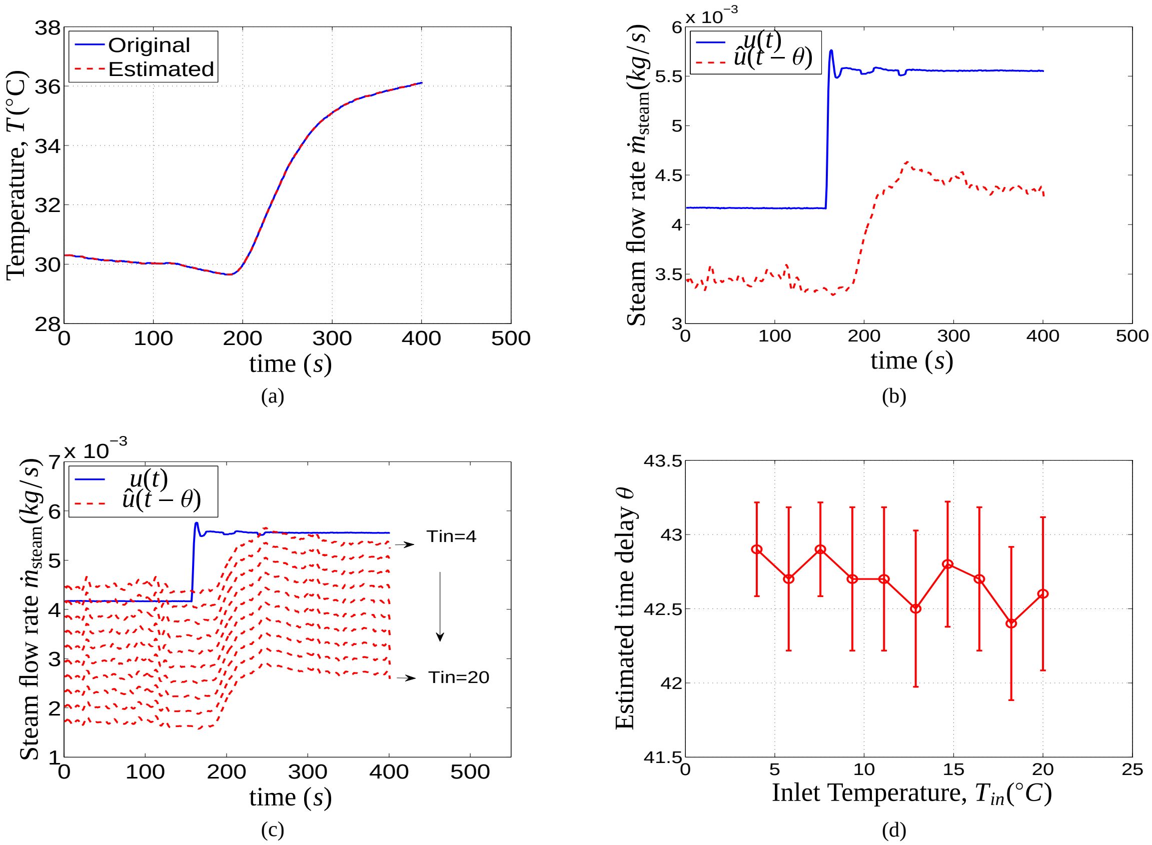

Figure 8: Validation of the Time Delay Estimation Algorithm using Open-Loop Experimental Data. (a) Estimation of the Temperature T (b) Estimation of the steam flow rate $\dot{m}_{\mathrm{steam}}$ when T_{in} is set to 10. (c) Estimation of the steam flow rate $\dot{m}_{\mathrm{steam}}$ when T_{in} is varying in the range $[4, 20]$. (d) Estimation of time delay θ for different T_{in} values.

6.4. Comparison of the Proposed Method with other Methods for the Experimental Data

Table 7 summarizes the different time delay values obtained from the three different experimental cases, as well as the values obtained using the direct time delay estimation method and an ARMAX-based search. It should be noted that the cross-correlation method will fail for all three examples, since none of the assumptions are fulfilled. Similarly, the step test method can only determine a time delay if a step change in either the input or reference signal has been performed. Therefore, the step test method cannot work for the routine operating case, since there are no such changes. On the other hand, the ARMAX-based search method provided reasonable estimates of the time delay. However, the exact value obtained does depend strongly on the model orders selected. Note that now there is no real discernible difference between the two model order selections. Similarly, the Laguerre-model-based approach provides estimates for all three situations. It should be noted that for this system based on many different experiments and analysis of the results, it seems that a time delay of approximately 45 s is reasonable [18, 20]. It can be seen that, except for the ARMAX-based search method, all examined approaches provide reasonable values, when the given method is applicable. It should be noted that with the ARMAX-based search method, as in any such method, the amount of time required to search for a solution can increase drastically. Such a problem is not encountered in the proposed method, whose complexity depends solely on the size of the differential equation.

7. Conclusions

This paper has examined the problem of estimating the time delay for a chemical process given different types of process data: open-loop, closed-loop with reference signal excitation, and closed-loop without reference signal

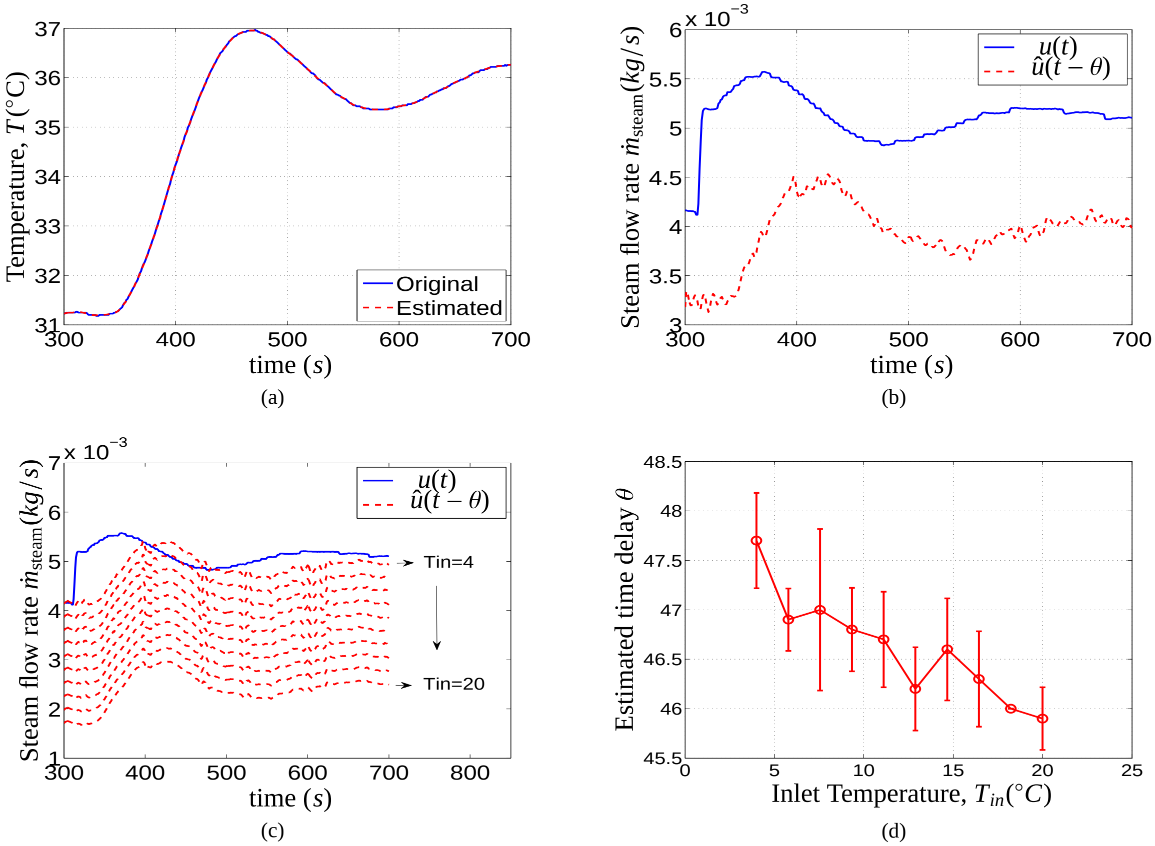

Figure 9: Validation of the Time Delay Estimation Algorithm using Closed-Loop Experimental Data with Reference Signal Excitation (a) Estimation of the Temperature T (b) Estimation of the steam flow rate $\dot{m}_{\text{steam}}$ when T_{in} is set to 10. (c) Estimation of the steam flow rate $\dot{m}_{\text{steam}}$ when T_{in} is varying in the range $[4, 20]$. (d) Estimation of time delay θ for different T_{in} values.

excitation, that is, routine operating data. The time delay estimation was performed using a least squares support vector machine method that converts the solution of the differential equations into an optimization of a set of algebraic equations. Such an approach has the advantage that the method does not require multiple integrations in order to obtain a solution. This approach was tested on both simulations of and historical data obtained from a heated tank system.

The results showed that the proposed method can easily estimate the correct time delay irrespective of signal-to-noise ratio or unmeasured additive disturbances. This observation is very important as it is common in chemical processes to have some unmeasured factors that can influence the overall system. Therefore, since this method is not influenced by these parameters, it can be used even if complete information about the process is unavailable. It would be useful to now test this proposed approach on more complex systems with greater uncertainties and unmeasured parameters.

Subsequent work seeks to apply this approach to more complex and involved chemical systems, such as a distillation column. As well, it is necessary to determine the implications of identifiability, that is, determining the required persistent excitation of the input signal, on time delay identification.

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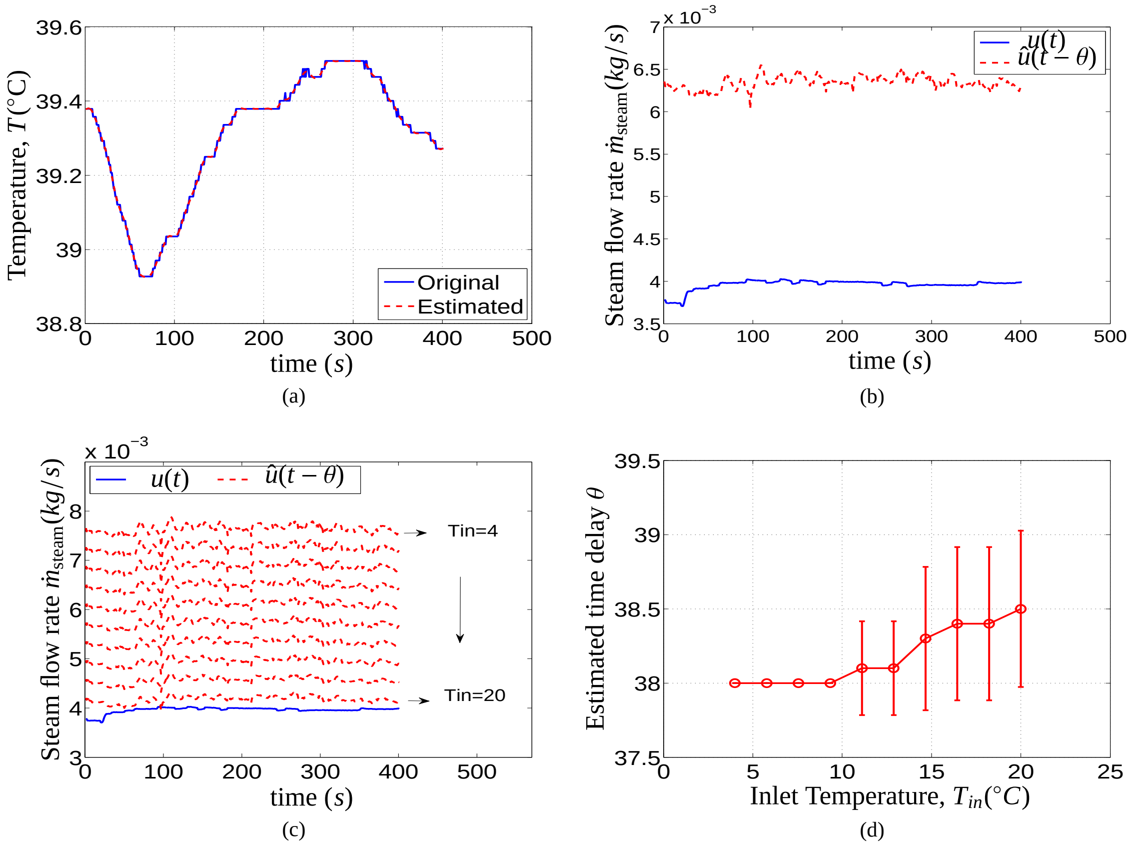

Figure 10: The results of the closed-loop-2 case dataset. (a) Estimation of the Temperature T (b) Estimation of the steam flow rate $\dot{m}_{\text{steam}}$ when T_{in} is set to 10. (c) Estimation of the steam flow rate $\dot{m}_{\text{steam}}$ when T_{in} is varying in the range $[4, 20]$. (d) Estimation of time delay θ for different T_{in} values.

Table 7: Comparing the Performance of the Proposed Method, the Direct Step Test Values, the ARMAX-based search implemented by MATLAB's DELAYEST, and Laguerre Methods for Estimating the Time Delay Using Experimental Data

	Method				
	Step Test	DELAYEST		Laguerre Method	Proposed
Data Set		Model Order = 1	Model Order = 10		
Open-Loop Example	45	35	32	31	43
Closed-Loop Example	38	40	39	42	46
Routine Operating Data Example	N.A.	24	35	24	38

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